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Resolving collisions in Stokes suspensions with an efficient and stable potential-free constrained optimization algorithm WEN YAN, Center for Computational Biology, Simons Foundation, EDUARDO CORONA, SHRAVAN VEERAPANENI, Department of Mathematics, University of Michigan, MICHAEL SHELLEY, Center for Computational Biology, Simons Foundation and Courant Institute of Mathematical Sciences — A common challenge in simulating dense suspension of rigid particles in Stokes flow is the numerical instability that arises due to particle collisions. To overcome this problem, often a strong repulsive potential between particles is prescribed. This in turn leads to numerical stiffness and dramatic reduction in stable time-step sizes. In this work, we eliminate such stiffness by introducing contact constraints explicitly and solving the hydrodynamic equations in tandem with a linear complementarity problem with inequality constraints. The Newton's third law of the collision force is explicitly guaranteed to allow consistent calculation of collision stresses. Efficient parallelization for shared-memory and distributed-memory architectures is also implemented. This method can be coupled to any Stokes hydrodynamics solver for particles with various shapes and allows us to simulate $10^4 \sim 10^7$ spheres on a laptop, depending on the cost of the Stokes hydrodynamics solver. We demonstrate its performance on a range of applications from active matter to multi-physics problems.

Wen Yan
Center for Computational Biology, Simons Foundation

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